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THE FUNDAMENTAL SOLUTION OF THE HEAT EQUATION ON A COMPACT LIE GROUP

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1. Introduction

The purpose of this paper is to study the fundamental solution of the heat equation on a compact Lie group. Our main result is to express this function in terms of a product over the roots of the Lie group. The terms in this product are then identified as classical functions. The result is the following.

Theorem 1.1. *Let G be a compact semisimple, simply connected Lie group. Then the fundamental solution of the heat equation is*

$$K(x,t) = \frac{\operatorname{vol} G e^{(2\mu+l)t/24}}{\pi^{2(2\mu+l)/3} 2^{2(\mu+l)/3+\mu}} \left(-\theta'(t/8)\right)^{-(\mu-l)/3} \times \prod_{\alpha>0} -\frac{\theta_3'(\pi\alpha(x)/2, it/8\pi)}{\sin \pi\alpha(x)}.$$

The notation in this theorem is the following. Firstly,

$$\theta(t) = \sum e^{-n^2 t} \tag{1.1}$$

with the sum over all integers and $\theta'(t)$ is the usual derivative of θ. Then

$$\theta_3'(z,t) = \frac{\partial\theta_3}{\partial z}(z,t) \tag{1.2}$$

where θ_3 is the classical theta function of [5]. Notice that we are using t for the second variable rather than $q = e^{i\pi t}$ which is used in [5]. The constant μ is the number of positive roots and l is the rank of the Lie group.

The trace of the heat kernel is $K(1,t)$, where 1 is the identity element of the group. It follows immediately from Theorem 1.1 that we can express $K(1,t)$ in terms of classical functions.

Corollary 1.2. *The trace of the heat kernel is*

$$K(1,t) = \frac{\operatorname{vol} G e^{(2\mu+l)t/24}}{\pi^{2(2\mu+l)/3} 2^{2(2\mu+l)/3}} \left(-\theta'(t/8)\right)^{(2\mu+l)/3}.$$

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It is interesting to compare this with the Macdonald's identities. The fundamental solution solves the problem

$$(1.3) \qquad \Delta u + \partial u/\partial t = 0 \quad \text{and} \quad \lim_{t\to 0} u(x,t) = \delta_1(x),$$

where δ_1 is the Dirac delta distribution which is concentrated at the identity element of G. On the other hand let $K_a(x, t)$ solve the problem

$$(1.4) \qquad \Delta u + \partial u/\partial t = 0 \quad \text{and} \quad \lim_{t\to 0} u(x,t) = \delta_a(x),$$

where δ_a is the delta distribution concentrated on the orbit under conjugation of a, a special element called "principal of type ρ". The Macdonald's identities correspond to the formula

$$(1.5) \qquad K_a(1,t) = e^{-\dim G t/24}\eta(t)^{\dim G}.$$

This is explained in [1]. The point is that $K_a(1, t)$ is expressed in terms of a modular form: the Dedekind η-function.

The function $\theta(t)$ is also a modular form, see [4]. Now since $K(1, t)$ has a nontrivial asymptotic expansion it cannot be a modular form. However, Corollary 1.2 expresses $K(1, t)$ in terms of derivatives of modular forms. It happens that a product of modular forms is again a modular form. Derivatives of modular forms do not have this property. This means that $K(1, t)$ is a much more complicated function than $K_a(1, t)$.

This complication is even more pronounced when one compares $K(x, t)$ with $K_a(x, t)$. The formula for K_a which is analogous to that given in Theorem 1.1 is

$$(1.6) \qquad K_a(x,t) = \prod_{n=1}^{\infty} \det(1 - e^{-nt} Adx).$$

The reader is referred to [1] for details on the results concerning K_a.

This paper pursues the argument of [1] but in the more complicated case of the fundamental solution. In the next section we consider the case of SU(2) and describe some of the classical functions. The third section describes the product over the positive roots and the final section explores the relationship with the asymptotic expansions.

Added in proof. In the special case of $G = \mathrm{SU}(2) \approx S^3$, this result is given in the paper by J. Cheeger and M. Taylor, *On the diffraction of waves by conical singularities*. I, Comm. Pure Appl. Math. **35** (1982) 295.

2. The heat equation and classical functions

In this section we shall calculate the fundamental solution of the heat equation on the group SU(2). The main point of this is to relate this solution to the classical theta functions. We shall also describe the asymptotic expansion of the trace of the heat kernel.

To begin we describe the representation theory of SU(2). The space of dominant weights is taken as

$$D = \{\lambda : 2\lambda \in \mathbf{Z}, \lambda \geqslant 0\}. \tag{2.1}$$

Then for $\lambda \in D$ there is a character χ_λ which is given by the Weyl character formula as

$$\chi_\lambda(x) = \sin(2\lambda + 1)\pi x / \sin \pi x. \tag{2.2}$$

This is the trace of the representation π_λ on the space V_λ, which has dimension

$$\dim V_\lambda = 2\lambda + 1. \tag{2.3}$$

In these formulae x is an element of the circle S^1 which is taken as the maximal torus of SU(2).

We need the eigenvalues of the Laplacian. These are given by

$$\Delta \chi_\lambda = c(\lambda)\chi_\lambda \tag{2.4}$$

with

$$c(\lambda) = \tfrac{1}{2}\lambda(\lambda + 1). \tag{2.5}$$

Now we can write down the fundamental solution of the heat equation. By using the Peter-Weyl theorem this can be written as a series in characters:

$$K_3(x, t) = \sum_{\lambda \in D} (2\lambda + 1)\frac{\sin(2\lambda + 1)\pi x}{\sin \pi x} e^{-\lambda(\lambda+1)t/2}. \tag{2.6}$$

Setting $n = 2\lambda + 1$ allows this to be written as

$$K_3(x, t) = \sum_{n=1}^{\infty} n\frac{\sin n\pi x}{\sin \pi x} e^{-(n^2-1)t/8}. \tag{2.7}$$

Our aim is to identify this solution in terms of the classical functions. The appropriate function is $\theta_3(z, t)$, see [5], and is defined as

$$\theta_3(z, t) = 1 + 2\sum_{n=1}^{\infty} \cos 2nz e^{i\pi n^2 t}. \tag{2.8}$$

Hence differentiating with respect to z gives

$$\frac{\partial \theta_3}{\partial z}(z, t) = \theta_3'(z, t) = -4\sum_{n=1}^{\infty} n \sin 2nz e^{i\pi n^2 t}. \tag{2.9}$$

It is now easy to identify K_3 in terms of θ_3. We state the result as follows.

Proposition 2.1. *The fundamental solution of the heat equation on* SU(2) *is*

$$K_3(x, t) = \frac{-e^{t/8}}{4 \sin \pi x}\theta_3'(\pi x/2, it/8\pi).$$

The next result we shall need is to identify $K_3(1, t)$. Here 1 denotes the identity element of the group SU(2). In the notation we have chosen for the maximal torus the identity element corresponds to taking $x = 0$.

Proposition 2.2. *At the identity element* $1 \in \mathrm{SU}(2)$ *the fundamental solution is*

$$K_3(1, t) = -\tfrac{1}{2}e^{t/8}\theta'(t/8)$$

where $\theta(t) = \sum_{n=-\infty}^{\infty} e^{-2t}$ *and* $\theta' = \partial\theta/\partial t$.

Proof. From equation (2.7) and L'Hopital's rule we see that

$$K_3(1, t) = \sum_{n=1}^{\infty} n^2 e^{-(n^2-1)t/8}, \tag{2.10}$$

Now

$$\theta'(t) = -2 \sum_{n=1} n^2 e^{-n^2 t}, \tag{2.11}$$

and the result of the proposition follows immediately.

It happens that $\theta(t)$ is, up to a change of notation, a modular form of weight one half. The transformation equation is (see [4])

$$\theta(t) = (t/\pi)^{-1/2}\theta(\pi^2/t). \tag{2.12}$$

If we differentiate (2.12) we obtain

$$\theta'(t) = -(t/\pi)^{-5/2}\theta'(\pi^2/t) - \tfrac{1}{2}\pi^{1/2}t^{-3/2}\theta(\pi^2/t). \tag{2.13}$$

We can use these transformation laws to give the asymptotic expansion of $K_3(1, t)$. If we neglect exponentially small terms we see

$$\theta(t) \sim 1 \quad \text{as } t \to \infty \tag{2.14}$$

and

$$\theta'(t) \sim 0 \quad \text{as } t \to \infty. \tag{2.15}$$

Thus from (2.12) we see

$$\theta(t) \sim (t/\pi)^{-1/2} \quad \text{as } t \to 0, \tag{2.16}$$

and from (2.13)

$$\theta'(t) \sim -\tfrac{1}{2}\pi^{1/2}t^{-3/2} \quad \text{as } t \to 0. \tag{2.17}$$

Combining these results with the previous proposition gives the asymptotic expansion for the trace of the heat kernel.

Proposition 2.3. *The asymptotic expansion of the trace of the heat kernel is*

$$K_3(1, t) \sim 32\sqrt{2}\,\pi^2(4\pi t)^{-3/2}e^{t/8} \quad \text{as } t \to 0.$$

Here $e^{t/8}$ *represents the series* $1 + t/8 + (t/8)^2/2! \cdots$.

Corollary 2.4. *The volume of the group* SU(2) *with respect to the Killing form metric is* $32\sqrt{2}\,\pi^2$.

Proof. The usual asymptotic expansion (see [2]) is

$$K_3(1, t) \sim \operatorname{vol} G(4\pi t)^{-3/2} e^{t/8} \quad \text{as } t \to 0.$$

Now equating the two expansions gives the result in the corollary.

3. The fundamental solution as a product

In this section we shall establish a product formula for the fundamental solution of the heat equation. This is analogous to the product formula of [1] and the reader is referred to [1] for some of the details. We begin by recalling the definition of the fundamental solution and its reduction to the maximal torus.

The fundamental solution of the heat equation $K(x, t)$, is the solution of the following problem:

$$\Delta K + \partial K/\partial t = 0, \quad \lim_{t\to 0} K(x, t) = \delta_1(x). \tag{3.1}$$

Here $\delta_1(x)$ is the Dirac delta distribution concentrated at the identity element of G. Notice that the Laplacian, Δ, has had its sign chosen so that it has an increasing sequence of positive eigenvalues.

The reduction of K to the maximal torus is $K_T(x, t)$. This is given by

$$K_T(x, t) = \exp\left(-\|\rho\|^2 t\right) j(x) K(x, t), \tag{3.2}$$

where ρ is half the sum of the positive roots, $\| \, \|^2$ is the square of the Killing form norm and $j(x)$ is the denominator function

$$j(x) = \prod_{\alpha>0} 2i \sin \pi\alpha(x). \tag{3.3}$$

The reason for considering this reduction, rather than the more obvious restriction, is that K_T is a solution of the flat heat equation on the maximal torus T.

Proposition 3.1. *The function* K_T *solves the heat problem* $\Delta_T K_T + \frac{\partial K_T}{\partial t} = 0$, $\lim_{t\to 0} K_T(x, t) = \nu(x)$ *on the torus* T *where*

$$\nu(x) = \sum_{\lambda\in P} \prod_{\alpha>0} \frac{\langle \lambda, \alpha \rangle}{\langle \rho, \alpha \rangle} \exp(2\pi i \lambda(x)).$$

Proof. That K_T satisfies the heat equation is a simple consequence of a result of Harish-Chandra. This is

$$j(x)(\Delta f)(x) = \left(\Delta_T - \|\rho\|^2\right) j(x)(f|T)(x) \tag{3.4}$$

and may be found in [3].

The main interest of this proposition is the identification of the distribution ν. Let

$$d(\lambda) = \prod_{\alpha>0} \langle \lambda, \alpha\rangle / \langle \rho, \alpha\rangle. \tag{3.5}$$

Then by the Peter-Weyl theorem

$$K(x,t) = \sum d(\lambda+\rho)\chi_\lambda(x)\exp\left(-\|\lambda+\rho\|^2 t + \|\rho\|^2 t\right). \tag{3.6}$$

Here the sum is over the weights λ in the dominant Weyl chamber. Now, using the Weyl character formula, we obtain

$$\begin{aligned} &K_T(x,t) \\ &= \sum_\lambda \prod_{\alpha>0} \frac{\langle \lambda+\rho, \alpha\rangle}{\langle \rho, \alpha\rangle} \sum_w (-1)^w \exp(2\pi i w(\lambda+\rho)x)\exp\left(-\|\lambda+\rho\|^2 t\right). \end{aligned} \tag{3.7}$$

The sum over λ is the same as in (3.6) while the second sum is over w in the Weyl group. Thus the distribution ν is

$$\nu(x) = \sum_\lambda \prod_{\alpha>0} \frac{\langle \lambda, \alpha\rangle}{\langle \rho, \alpha\rangle} \sum_w (-1)^w \exp(2\pi i w(\lambda)x). \tag{3.8}$$

This is the equivalent to the result of the proposition.

We shall make some comments to explain why (3.8) is equivalent to the result of the proposition. The difference between $\{\lambda+\rho\}$ and $\{\lambda\}$ for λ a dominant weight is just the set of weights in the walls of the Weyl chamber. Since $\prod\langle\lambda,\alpha\rangle = 0$ for such weights we can remove "ρ" from (3.7). To change the sum, from over the dominant weights and Weyl group to over all the weights, we use the invariance of the Killing form under the Weyl group. Again we introduce repetitions for weights in the walls of the Weyl chambers but these do not contribute to the sum.

For convenience we call K_T the associated fundamental solution and ν the associated delta distribution. The purpose of these associated objects is to pass from the Lie group to the torus where it is easier to carry out the analysis. We shall, therefore, transfer our results to the maximal torus, prove them and then lift the answers back to the group.

Theorem 3.2. *Let K_3 denote the fundamental solution of the heat equation on* SU(2). *Then there is a function $F(t)$ such that $K(x,t) = F(t)\prod_{\alpha>0} K_3(\alpha(x), t)$.*

Proof. This follows the same argument that was used in [1]. To start with we restate the result in terms of the associated functions. Then we see that it is sufficient to show

$$K_T(x,t) = e^{(\mu-l)t/24}F(t)\prod_{\alpha>0} K_{3T}(\alpha(x),t). \tag{3.9}$$

Here μ is the number of positive roots, l is the rank of G and K_{3T} is the associated fundamental solution on SU(2).

To prove (3.9) we pick an ordering $\alpha_1,\cdots,\alpha_\mu$ of the positive roots and embed T in the μ-dimensional torus T^μ by

$$A\colon T\to T^\mu,\quad A(x) = \big(\alpha_1(x),\cdots,\alpha_\mu(x)\big). \tag{3.10}$$

Let $T^\perp$ be the subspace of T^μ which is orthogonal to T. Then the fundamental solution on T^μ is the product of the fundamental solutions on T and $T^\perp$. Denoting by H, $H_\perp$ and H_μ respectively the fundamental solutions on T, $T^\perp$ and T^μ we have

$$H_\mu(z,t) = H(x,t)H_\perp(y,t) \tag{3.11}$$

where $z = x + y$.

To pass from the fundamental solution, H, to the associated fundamental solution, K_T, requires convolution with the associated delta distribution. In Proposition 3.1 we identified the Fourier transform of ν as

$$\tilde{\nu}(\lambda) = \prod_{\alpha>0} \langle\lambda,\alpha\rangle/\langle\rho,\alpha\rangle. \tag{3.12}$$

Thus, up to a constant $\nu(x)$ is the convolution of the distributions $\nu_3(\alpha(x))$:

$$\nu(x) = C\nu_3\big(\alpha_1(x)\big) * \cdots * \nu_3\big(\alpha_\mu(x)\big). \tag{3.13}$$

We can identify C as

$$C = \prod_{\alpha>0} 1/(4\langle\rho,\alpha\rangle) \tag{3.14}$$

with the factor $1/4$ occurring since $\prod_{\alpha>0}\langle\rho,\alpha\rangle = 1/4$ for the group SU(2). We extend ν to the whole of T^μ by

$$\nu_\mu(z_1,\cdots,z_\mu) = C\nu_3(z_1) * \cdots * \nu_3(z_\mu). \tag{3.15}$$

Now taking convolutions with the left-hand side of (3.11) gives the function

$$C\prod_{j=1}^{\mu} K_{3T}(z_j). \tag{3.16}$$

On the other hand we can identify ν_μ as a delta distribution. This is

$$\nu_\mu = C\prod_{j=1}^{\mu} 2i\sin\pi z_j\delta_1. \tag{3.17}$$

So taking convolutions with the right-hand side of (3.11) gives the function

$$K_T(x,t)K^{\perp}{}_T(y,t). \tag{3.18}$$

Now setting $z = x$ so $z_j = \alpha_j(x)$ and $y = 0$ gives the result in the theorem with

$$e^{(\mu-l)t/24}F(t) = C/K^{\perp}{}_T(0,t). \tag{3.19}$$

4. The fundamental solution and its asymptotic expansion

The purpose of this section is to collect together the results of the previous sections, and so give the expression for the fundamental solution of the heat equation in terms of the classical theta functions. After we have done this we shall investigate the asymptotic expansion of the trace of the heat kernel.

Theorem 4.1. *Let G be a compact semisimple, simply connected Lie group. Then the fundamental solution of the heat equation is*

$$K(x,t) = \frac{\operatorname{vol} G e^{(2\mu+l)t/24}}{\pi^{2(2\mu+l)/3}2^{2(2\mu+l)/3+\mu}}(-\theta'(t/8))^{-(\mu-l)/3}$$
$$\times \prod_{\alpha>0}\frac{-\theta_3'(\pi\alpha(x)/2, it/8\pi)}{\sin\pi\alpha(x)}.$$

Proof. By Theorem 3.2 we have

$$K(x,t) = F(t)\prod_{\alpha>0}K_3(\alpha(x),t). \tag{4.1}$$

Now we need to identify $F(t)$. By (3.19)

$$e^{(\mu-l)t/24}F(t) = C/K^{\perp}{}_T(0,t) \tag{4.2}$$

for a constant $C = \prod_{\alpha>0}1/(4\langle\rho,\alpha\rangle)$. Thus $F(t)$ is given in terms of the solution to the heat equation. If we pass from the associated solutions to fundamental solutions on G we obtain

$$F(t) = k(K_3(1,t))^{-(\mu-l)/3}. \tag{4.3}$$

Notice that $\mu - l$ is the dimension of $T^{\perp}$ and K_3 is the fundamental solution on the three dimensional manifold SU(2). Recall the formulae for $K_3(1,t)$ and $K_3(x,t)$:

$$K_3(1,t) = -\tfrac{1}{2}e^{t/8}\theta'(t/8) \tag{4.4}$$

and

$$K_3(x,t) = -e^{t/8}\theta_3'(\pi x/2, it/8\pi)/4\sin\pi x. \tag{4.5}$$

Upon substituting these into (4.3) and (4.1) we obtain

$$(4.6)\quad K(x,t) = he^{(2\mu+l)t/24}(-\theta'(t/8))^{-(\mu-l)/3} \prod_{\alpha>0} -\frac{\theta_3(\pi\alpha(x)/2, it/8\pi)}{\sin\pi\alpha(x)},$$

for some constant h. To determine h we use the asymptotic expansion for $K(1,t)$. From [2] this is

$$(4.7)\qquad K(1,t) \sim (4\pi t)^{-\dim G/2} \operatorname{vol} G e^{(2\mu+l)t/24}.$$

Now we have already shown that

$$(4.8)\qquad \theta'(t) \sim -\tfrac{1}{2}\pi^{1/2}t^{-3/2}.$$

Using this formula gives a value for the constant h as

$$(4.9)\qquad h = \operatorname{vol} G/\pi^{2(2\mu+l)/3}2^{2(2\mu+l)/3+\mu}$$

which completes the proof of the theorem.

Some comments are required on this method of determining the constant h. It is clear that

$$(4.10)\qquad h = k(1/2)^{-(\mu-l)/3}(1/4)^{\mu}$$

so determining h is essentially the same as determining k. From (4.3) it is clear that k is related to C. On the other hand (4.9) gives an expression for h in terms of the volume of G. Thus if we could determine k directly we would obtain a value for the volume of G.

The difficulty here is in comparing the measures on the different spaces involved. The measure on T is related to that on G by the Weyl integration formula. On the other hand T is embedded isometrically in T^{μ} and T^{μ} has the standard flat measure inherited from the Euclidean measure on $\mathbf{R}^{\mu}$. However, in (4.3) the constant k has absorbed a factor which relates the measure on $T^{\perp}$ to that on the product space $V^{\mu-l}$, where V is a line in the Lie algebra of SU(2). It is this factor which prevents us from equating k with C.

In [2] we obtained the asymiptotic expansion for the trace of the heat kernel by considering its expansion as a series in characters. This did indeed lead to a formula for the volume of G. This is

$$(4.11)\qquad \operatorname{vol} G = (2\pi)^{l+\mu}\operatorname{vol} Q(R^{v}) / \prod_{\alpha>0} \langle \rho, \alpha \rangle.$$

Now if we set $h = mc$ then we find

$$(4.12)\qquad m = 2^{(2\mu+l)/3}\pi^{(l-\mu)/3}\operatorname{vol} Q(R^{v}).$$

In both (4.11) and (4.12) the term $\operatorname{vol} Q(R^{v})$ is the volume of the fundamental parallelepiped of the lattice generated by the co-roots.

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